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13. ABSTRACT *(Maximum 200 Words)*

The theory and phase-field modeling of formation and deformation of adaptive nano-composites containing polydomain martensitic and ferroelastic layers are developed. It has been shown that superplastic and superelastic deformation of heterophase and polydomain martensite structures are reversible in the composites to the contrary to bulk shape memory materials. By the engineering of constraints, the controlled polydomain structures have designed and the characteristics of superelastic and superplastic giant deformation have been optimized. The theory has been applied to the formulation of principles of actuators with enhanced efficiency and efficacy. Two new models of layer actuators were developed based on: (1) manipulating a bend curvature by using combination of passive layers with coefficient of thermal expansions and (2) bending of the films transforming by the movement of martensite/austenite interface oriented along the film.

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THEORY AND MODELING OF ADAPTIVE NANOCOMPOSITES

Final Report

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Research Objectives

The research focuses on developing a new approach for materials engineering: using mescoscopic design of composites with transformable components (*adaptive composites*) to control self-assembling micro- and nano-structures arising during structure phase transformations. Such self-assembling polydomain structures are natural products of phase transformations in solids. The trend to minimize the energy of long-range elastic interactions leads to the formation of self-organized arrangements of domains of different phases or differently oriented domains of the same phases (twins). Transformations in bulk materials usually result in the formation of complex irregular polydomain structures that are difficult to control. In contrast, it is possible to obtain a completely controlled structure in a single crystalline film through constraint. The constraint can be imposed by embedding transformable materials in a composite architecture. Thus, the combination of engineered mesostructures and self-organized micro- and nano- polydomain structures presents broad opportunities to design new materials with well-controlled structures at multiple length scales. *The general goal of this research is to develop theoretical principles and computational tools to design materials with self-assembled micro- and nano-structures controlled through fabricating composite architectures.* To accomplish this goal, we started with developing the theory and modeling describing the formation of adaptive polydomain micro- and nano-structures through martensitic transformations in constrained thin films. Shape memory alloys, which change their polydomain microstructure in response to thermal or mechanical loading, have been chosen as model adaptive materials.

The proposed research will impact a variety of aerospace applications. For conventional aircraft, a new class of actuators and sensors can be developed for microdevices, being used to miniaturize existing systems. For newer aircraft concepts, such as morphing structures, curvature sensors and bending actuators can be developed for optimizing shape control.

Research accomplishments with references to corresponding publications are presented below.

Thermodynamic analysis of martensitic transformation in polydomain adaptive composite and superelastic deformation with controlled hysteresis

Superelastic deformation of shape memory alloys is a result of a polydomain microstructure evolution during stress-induced martensitic transformations. In bulk materials, the deformation is not reversible and proceeds with stress-strain hysteresis. Our thermodynamic analysis shows that in adaptive composites containing a shape-memory alloys as an active component can exhibit the reversible superelastic deformations with an absence of quasistatic hysteresis [1-3]. In the contrary to bulk materials where the transformations are locally inhomogeneous, the microstructure evolution in constraint single crystalline thin layer can be well-controlled (Fig.1). Therefore, the multilayer composite consisting of thin (<1μm) active layers separated by thin layers of a passive material allows one to obtain superelastic material with controlled deformation properties.

The superelastic deformation of shape memory alloys, even with perfect microstructure, is intrinsically unstable as a result of incompatibility between polytwin martensite and austenite phases at stress-induced and stress assistant transformations. This instability leads to the

thermodynamic stress-strain hysteresis of the superelastic deformation [4]. It has been shown that the combination of a shape memory active material with a non-transforming passive material can decrease and suppress the instability of superelastic deformation. The stability analysis of superelastic deformation allows one to formulate design principles of adaptive composites with controlled stress-strain hysteresis and potentially large reversible deformation (Fig.2) [3].

In ultra-thin nano-scale active layers the transformations proceeds through the formation of single –domain martensite with high mobility of martensite/austenite interfaces (Fig.1 path 3). Due to difficulty of dislocation nucleations in this heterophase nanostructure it is expected that some materials exhibit reversible martensite transformations and shape-memory effect, although they have no such properties in bulk. This heterophase polydomain structure is analyzed in [5,6,7].

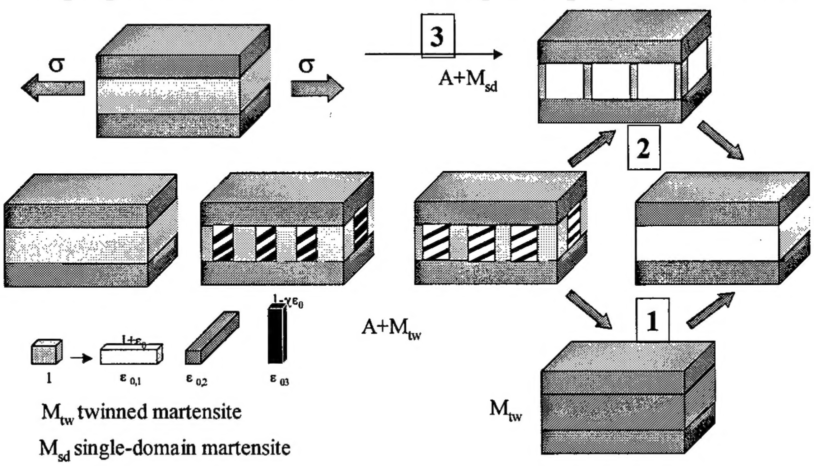

Figure 1: SMA active layer between two passive layers. Three paths of microstructure evolutions during stress induced transformations in a constrained layer: 1, 2- through the formation of polytwin martensite; 3- through the formation of single domain martensite.

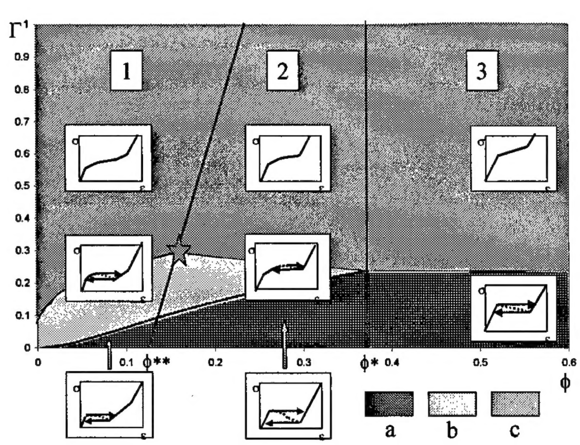

Figure 2: Diagram of stability of superelastic deformation of the composite, ϕ is an effective temperature (0 corresponds to the equilibrium phase temperature) , Γ is a constraint parameter , $\Gamma = (1+\gamma\psi)^{-1}$, γ is a ratio of fractions of active and passive layers, ψ is a ratio of the elastic moduli. Areas 1, 2, 3 correspond to three path of the transformation in Fig.1. The star corresponds to the hysteresisless deformation with maximum superelastic strain. a - superelastic deformation is stable. b- superelastic deformation is stable at yield stress. c- superelastic deformation is unstable.

Engineering of polydomain martensite structure and reversible superplastic deformation of martensite

The thermodynamic theory and phase-field modeling have been developed to describe formation and deformation of the adaptive composite containing polydomain (polytwin) layers of the martensite phase. It has been shown that it possible to engineer controlled polydomain structure by manipulating mechanical constrains: thickness, misfit, crystallographic orientations and elastic properties of composite layers [8-10]. The thermodynamic analysis of equilibrium microstructures with sharp interfaces allows us to determine an equilibrium domain fraction and preferable interface orientations between domains . The phase-field modeling was employed to determine polydomain architecture and its scale. As an example, Fig.3 presents polytwin structures arising at cubic-tetragonal phase transformation, which is quite generic and corresponds to different types of solid-solid structural transformations (order-disorder, ferroelastic and martensitic (including BCC-FCC transformations). Depending on the misfit between the layers two types of relaxed microstructure exist: hierarchical and cellular ones. Available experimental data on polydomain microstructures resulting from ferroelastic transformations in oxide epitaxial films support the result of modeling.

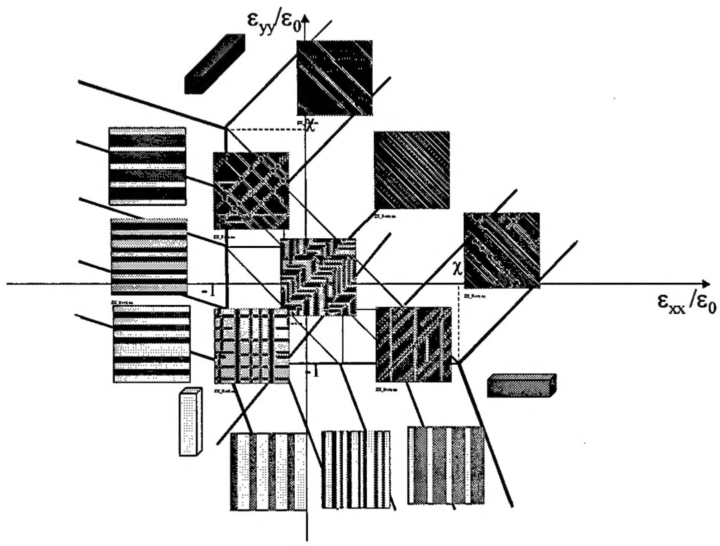

Figure 3: Phase-field modeling of the equilibrium polydomain structures dependent on biaxial misfit strain between layers: ε_{xx}, ε_{yy}. Three-domain architectures inside the triangle correspond to the complete relaxation of misfit stress, two-domain architectures outside the triangle are uniaxially stressed and single-domain layers near the vertices are biaxially stressed.

After the initial polydomain structure is obtained, the composite was uniaxially stressed and the equilibrium structure is studied as a function of an external stress. The example of reversible superplastic deformation which accompanied by transformation of three-domain structure, two-domain or single domain one is presented in Fig.4 [11]. The structure evolution considered above is driven by minimization of the elastic energy and therefore, it is typical for all structure transformations in solids. Particularly, the results of these simulations have been expanded to the evolution of ferroelectric polydomain structures under external electrical field. In this case the polydomain evolution leads to the giant piezoresponce [11].

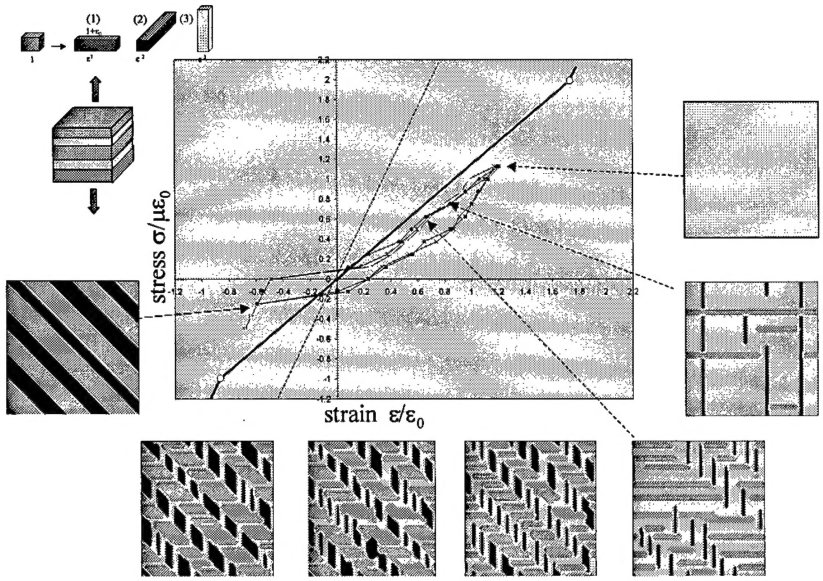

Figure 4: Superplastic deformation under stress normal to layers.

Bending of adaptive composites and theory of shape memory alloy actuators

The reversible superelastic and superplastic deformation of adaptive composites under uniform stress is limited by elasticity of passive layers. This limitation can be overcome if the bending mode of deformation is used. Therefore, thermodynamic analysis of stress-assistant martensitic transformation has been expanded to model superelastic deformation in a constrained film under bending. A bending SMA film is an active element in layer sensors and actuator responding to the change of temperature. A bimorph actuator (SMA film on a passive substrate) is considered in [12-14]. Two new models of layer actuators were explored based on

1. manipulating a bend curvature by using combination of passive layers with coefficient of thermal expansions.
2. bending of the films transforming by the movement of martensite/austenite interface oriented along the film.

1.The martensitic transformation in an active film of bimorph actuator consisting of a thin transforming layer and a thick substrate leads to relaxation of thermal stress due to layer misfit. Therefore, the stress in the active film cannot change its sign during the transformation and the curvature of the bimorph does not change its sign as well. However, it is possible to engineer an actuator with a curvature and a deflection changing its sign due to a transformation if a third layer with coefficient of thermal expansion less than the thermal expansion of substrate is interleaved. The theoretical model based on this idea has explained quantitatively the performance of composite membrane NiTi/SiO_2 on Si substrate.

2. A new concept of actuation presents the model of an active layer in which the transformation proceeds by the movement of a film plane parallel interface between initial and product phases (Fig.5)[14,15]. The bending of the film is a result of self-strain in a transformed part of the film. Calculation of the elastic energy of internal stresses show that there is an equilibrium position of

interface which can be shifted by a thermodynamic driving force. Thus, it is possible to obtain reversible movement of interface by changing temperature. Combining SMA film with top or/and bottom passive layers of different elastic properties, thickness and misfit it is possible to optimize the actuating deformation.

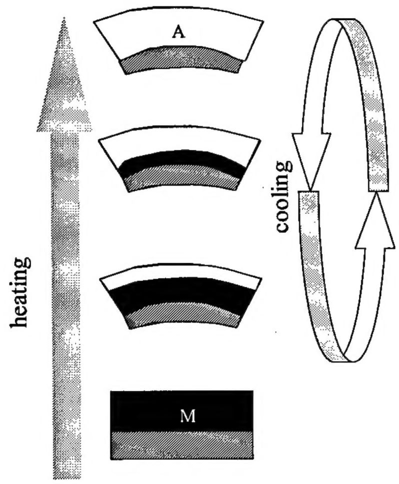

Figure 5: The reversible transformation in the film on the substrate after the martensite state in the film is reached under cooling.

The dynamics of actuators is determined by kinetics of interface movement which is quantitatively described by solving a Stefan-type problem with an equilibrium temperature at the interface between phases dependent on interface position. The computational technique has been developed to control dynamics of the actuator through the variation of temperature at the top and the bottom of the active layer.

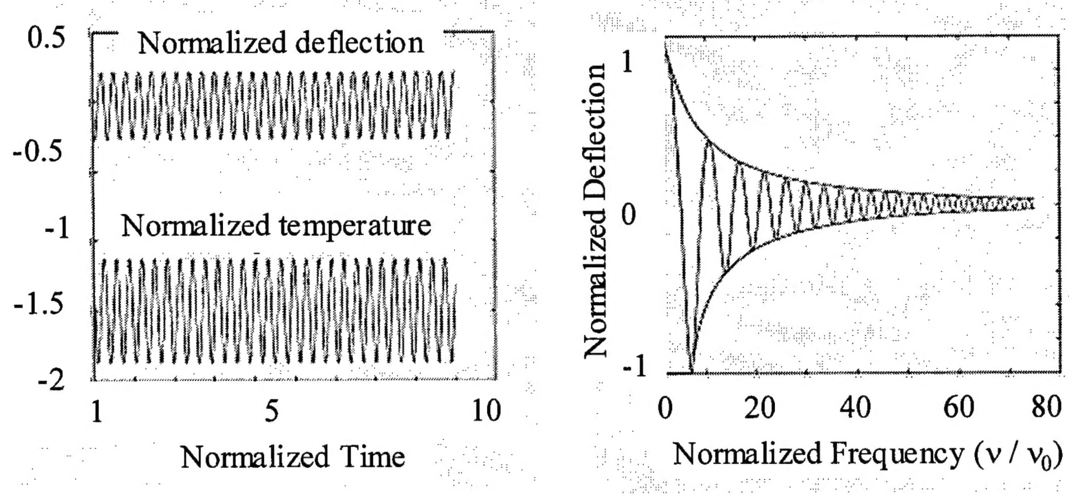

Figure 6. Periodic bending of SMA actuators under periodic change of surface temperature and the dependence of maximum deflection on temperature change frequency. $\nu_0 = \chi / 2L^2$ *, L is a thickness of an actuator,* χ *is a thermal diffusivity.*

In [14,15] has been shown that the reversible movement of interface leading to reversible bending of the plate is possible under cycling of uniform temperature of the plate (a two-way shape memory effect) (see Fig.5). Coupling this solution with heat diffusion equation allows one to describes the kinetics of bending as a function of control temperature of the top and bottom surfaces of the plate (Fig. 6). The periodic change of the surface temperature induces the periodic bending of the plate with the maximum deflection depending on the frequency of the temperature change. For a typical value of heat transfer coefficient, $\chi=10^{-4}$-10^{-5} m^2/s , the actuation frequency is approximately 100 Hz for a plate with thickness 1mm and may exceeds 1 MHz for thickness approaching 1 μm.

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Invited talks

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6. J.Slutsker and A.L.Roytburd , "Elastic Domain Microstructures in Epitaxial Layers", TMS 2003, San Diego, CA, March, 2003
7. A.L.Roytburd , "Nano- and Micro Elastic Domains in Constrained Ferroelastic Layers" TMS 2003, San Diego, CA, March, 2003
8. A.L.Roytburd, J.Slutsker and A.Artemev " Modeling of Composites with Self-Assembling Micro- and Nano-Structures ",TMS 2004, Charlotte, NC, March, 2004
9. A.L.Roytburd, "From Martensite to Self-Assembled Nanostructures", TMS 2004, Charlotte, NC, 2004.

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